Theory of Radio Frequency Spectroscopy of Polarized Fermi Gases

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We present two exact results for singular features in the radio frequency intensity $I(\omega)$ for ultracold Fermi gases. First, in the absence of final state interactions, $I(\omega)$ has a universal high frequency tail $C\omega^{-3/2}$ for *all* many-body states, where C is Tan's contact. Second, in a *normal* Fermi liquid at $T = 0$, $I(\omega)$ has a jump discontinuity of $Z/(1 - m/m^*)$, where Z is the quasiparticle weight and m^*/m the mass renormalization. We then describe various approximations for $I(\omega)$ in polarized normal gases. We show why an approximation that is exact in the $n_\downarrow = 0$ limit, fails qualitatively for $n_\downarrow > 0$: there is no universal tail and sum rules are violated. The simple ladder approximation is qualitatively correct for very small $n_\downarrow$, but not quantitatively.

There has been intense experimental activity on characterizing various states of matter in ultracold atomic gases [1, 2]. This will become ever more important with the possibility of new and exotic states being realized in these systems. An important tool in these studies is radio frequency (RF) spectroscopy where an RF pulse is used to transfer atoms from one hyperfine level to another. The RF signal [3, 4] has turned out to be much harder to interpret than initially thought because of complications of strong final state interactions and the inhomogeneity of trapped gases. Recently it has become possible to eliminate these problems by choice of suitable hyperfine levels (in ^{6}Li) and by tomographic techniques that focus on specific regions of the gas. The most detailed experimental results are available for polarized Fermi gases [5, 6].

Motivated by these experiments, we first describe two exact results for the *singular* features in RF spectra of a two-component Fermi gas with arbitrary interactions. Our results complement the exact results on sum rules [7, 8]. We work in the limit where final state interaction effects are negligible, so that we can focus on the nontrivial effects of interactions in the many-body state.

(1) The RF spectrum $I(\omega)$ has a universal $C\omega^{-3/2}$ tail at high frequencies, where C is Tan's contact coefficient [9], which is independent of spin. This form is valid for *all* phases of Fermi gases: superfluid [1, 2], highly imbalanced normal Fermi liquid [6, 10, 11, 12, 13] or even a balanced Galitskii Fermi Liquid [14].

(2) In any normal Fermi liquid state, the RF spectrum $I(\omega)$ at $T = 0$ has a jump discontinuity. Its location depends on the chemical potential μ and its magnitude is determined by the combination of Fermi liquid parameters $Z/(1 - m/m^*)$, where Z is the quasiparticle weight and m^* the effective mass.

These exact results are important not only in interpreting experiments, but also in understanding various approximation schemes [8, 15, 16], which are necessarily required to calculate the RF lineshape $I(\omega)$ for a strongly interacting gas. In the second part of our paper we critically analyze diagrammatic approximations for the highly imbalanced normal Fermi liquid.

(3) We show that a simple self-consistent approximation, motivated by the fact that it is essentially exact in the $n_\downarrow = 0$ limit [13], has serious qualitative problems for non-zero $n_\downarrow$: The minority spins do not exhibit the universal tail leading to sum rule violations and majority spins are completely unaffected.

(4) A simple ladder approximation, on the other hand, correctly exhibits all of the qualitative features expected on general grounds for $n_\downarrow > 0$, however there are quantitative inaccuracies and the approximation breaks down for $n_\downarrow \gtrsim 0.05$.

Formalism: Consider a Fermi gas with three hyperfine states which we label as $\uparrow$, $\downarrow$ and "e" (for excited or empty). The number density in levels $\sigma = \uparrow, \downarrow$ is n_σ with corresponding (non-interacting) Fermi energies $\epsilon_{F\sigma}$. The $\uparrow$ and $\downarrow$ fermions interact with an s-wave scattering length $a_{\uparrow,\downarrow} \equiv a$. The e-level is located at energy ΔE_σ from the bottom of the σ bands, and is empty ($n_e = 0$). We assume that fermions in the e state do not interact with those in σ levels: $a_{e,\sigma} \equiv 0$. If such interactions are strong, the simple results obtained below are considerably modified by vertex corrections [16]. One is then dealing with the complications of the probe in addition to the many-body system of interest.

When final state interactions are negligible linear response theory leads to the simple result:

$$I_\sigma(\omega) = \sum_{\mathbf{k}} A_\sigma(\mathbf{k}, \epsilon_{\mathbf{k}} - \mu_\sigma - \omega) n_F(\epsilon_{\mathbf{k}} - \mu_\sigma - \omega) \quad (1)$$

where the RF shift $\omega = \omega_{RF} - \Delta E_\sigma$, ω_{RF} is the RF frequency, $\epsilon_{\mathbf{k}} = k^2/2m$ is the bare dispersion, μ_σ the chemical potential, and $\hbar = 1$. $n_F(\epsilon)$ is the Fermi function and the single particle spectral function $A_\sigma(\mathbf{k}, \omega) = -\text{Im}G_\sigma(\mathbf{k}, \omega + i0^+)/\pi$ includes all many-body renormalizations due to interactions between $\uparrow$ and $\downarrow$ fermions.

Sum Rules and Large-ω behavior: The exact sum rules [7, 8] for the zeroth ($\ell = 0$) and first ($\ell = 1$) moments of the RF intensity $\int d\omega \omega^\ell I_\sigma(\omega)$, are valid for all values of a and $a_{e,\sigma}$. It might seem that the first moment sum rule (clock shift), which diverges as $a_{e,\sigma} \to 0$, can be of no use when final state interactions are negligible. However, we find that this divergence is actually related to a universal high frequency tail in $I_\sigma(\omega)$.

We rewrite (1) as $I_\sigma(\omega) = \sum_{\mathbf{k}} \int d\Omega A_\sigma(\mathbf{k}, \Omega) n_F(\Omega) \delta(\Omega - \epsilon_{\mathbf{k}} + \mu_\sigma + \omega)$. This

immediately leads to zeroth moment sum rule [17] $\int d\omega I_\sigma(\omega) = N_\sigma$, using $\int d\Omega A_\sigma(\mathbf{k}, \Omega) n_F(\Omega) = n_\sigma(\mathbf{k})$ and $\sum_\mathbf{k} n_\sigma(\mathbf{k}) = N_\sigma$ is the number of σ fermions.

We next analyze $I_\sigma(\omega \to \infty)$. The delta-function $\delta(\Omega - \epsilon_\mathbf{k} + \mu_\sigma + \omega)$ then contributes in one of two ways: either (a) Ω is large negative with $\epsilon_\mathbf{k}$ small, or (b) Ω small but $\epsilon_\mathbf{k}$ large. In case (a), however, the spectral function A_σ vanishes for small $\mathbf{k}$ and $\Omega \to -\infty$. Thus only case (b) survives and we find $I_\sigma(\omega \to \infty) \simeq \sum_\mathbf{k} n_\sigma(\mathbf{k})\delta(\epsilon_\mathbf{k} - \omega)$. Using Tan's result [9] $n_\sigma(\mathbf{k}) \simeq C/k^4$ for $k \gg k_F$ we thus find that

$$I_\sigma(\omega \to \infty) \approx \frac{1}{4\pi^2\sqrt{2m}}C\omega^{-3/2}, \qquad (2)$$

where C is the contact. We emphasize that the form of this result is independent of the phase (normal or superfluid) of the Fermi gas, though the value of C does depend on the phase. (This tail is absent only for the *noninteracting* gas for which $C \equiv 0$.) Note that this high frequency tail arises from short-distance physics in any Fermi gas, and is crucial for enforcing the *divergent* clock shift for $a_{e,\sigma} = 0$.

Fermi liquid singularity: In the study of many-body systems, various phases are often directly identified by characteristic low-energy singularities in measurable quantities, such as the the discontinuity at k_F in the momentum distribution of a Fermi liquid, or the square root singularity in the density of states of a s-wave superconductor at $T = 0$. Here we ask if any such singularity exists in the RF signal. Given the $\mathbf{k}$-sum and the kinematics in eq. (1), we see that there is no characteristic singularity in the paired superfluid state. However, as we show next, there *is* a singular signature for normal Fermi liquids at $T = 0$.

In the remainder of this paper we focus on the *normal* (i.e., non-superfluid) ground state of the highly polarized Fermi gas. Thus our results are relevant, e.g., to the unitary gas which has been predicted to be a normal Fermi liquid for $x = n_\downarrow/n_\uparrow < 0.4$, based on quantum Monte Carlo simulations [12]. (Our general results apply equally well to the dilute repulsive gas of Galitskii [14], which is yet to be realized in the laboratory.)

For a Landau Fermi liquid the spectral function is

$$A(\mathbf{k}, \omega) \simeq Z\delta\left(\omega - k_F(k - k_F)/m^*\right) + A^{\text{inc}}(\mathbf{k}, \omega) \quad (3)$$

close to the Fermi surface ($k \simeq k_F, \omega \simeq 0$). The subscript σ is dropped for simplicity. The first "coherent" term gives the quasiparticle pole in the Green's function with quasiparticle weight Z and effective mass m^* [18]. k_F is unshifted from its bare value as required by Luttinger's theorem [14]. The second non-singular term is the "incoherent" part of the spectral function.

The *singular* contribution to $I(\omega)$ is obtained by substituting the coherent term in (3) into (1) and using $n_F(\epsilon) = \Theta(-\epsilon)$ at $T = 0$. We convert the $\mathbf{k}$-sum to an integral over $\epsilon_\mathbf{k}$ and write the quasiparticle dispersion as $k_F(k - k_F)/m^* \simeq (k^2 - k_F^2)2m^* = (\epsilon_\mathbf{k} - \epsilon_F)m/m^*$.

For $m^* > m$ we find a peak which grows like a square root in ω and then has discontinuous drop, all of which rides on top of top of the smooth contribution from the incoherent piece. The location of the discontinuity ω^* and the size of the jump ΔI are thus given by [19]

$$\omega_\sigma^* = \epsilon_{F\sigma} - \mu_\sigma; \qquad \Delta I_\sigma = \frac{Z_\sigma N(\epsilon_{F\sigma})}{(1 - m/m_\sigma^*)}, \qquad (4)$$

where $N(\epsilon_{F\sigma})$ is the density of states at the Fermi energy.

Diagrammatic Lineshape Calculations: The form of the Fermi surface singularity and the high energy tail in the RF intensity have been elucidated above on general grounds. Calculating the detailed lineshape $I(\omega)$ necessarily requires approximations to be made for a strongly interacting Fermi system. Here we describe diagrammatic calculations for the highly imbalanced normal gas, highlighting the successes and limitations of two approximation schemes. All such calculations sum particle-particle (p-p) channel ladder diagrams: $\Gamma^{-1}(\mathbf{q}, iq_\ell) = m/4\pi a - \sum_\mathbf{k}\left[1/2\epsilon_\mathbf{k} - \beta^{-1}\sum_n G_\uparrow(\mathbf{k}+\mathbf{q}, ik_n + iq_\ell)G_\downarrow(-\mathbf{k}, -ik_n)\right]$. The rationale for focusing on p-p ladders can be given in many different ways. These are the leading diagrams for Fermi systems with short-range interactions in the low density repulsive Fermi liquid [14], in the Nozieres-Schmitt-Rink analysis [20] of the normal state of the BCS-BEC crossover, and in the $1/N$ expansion for the attractive Fermi gas [15].

One can analytically obtain closed-form expressions for the real and imaginary parts of the retarded $\Gamma^{-1}(\mathbf{q}, \omega + i0^+)$ when G_σ are the *bare* Green's functions; details are omitted for simplicity [21]. Next, the self-energies $\Sigma_\sigma(\mathbf{k}, ik_n) = \beta^{-1}\sum_{\mathbf{q},\ell}\Gamma(\mathbf{q}, iq_\ell)G_{-\sigma}(-\mathbf{k} + \mathbf{q}, -ik_n + iq_\ell)$ are calculated [22] using the spectral representation for the p-p vertex in terms of $\text{Im}\Gamma(\mathbf{q}, \omega + i0^+)$ to obtain $\Sigma_\sigma(\mathbf{k}, \omega + i0^+) = \Sigma_\sigma' + i\Sigma_\sigma''$. This in turn leads to the spectral functions $A_\sigma(\mathbf{k}, \omega) = -\text{Im}\left[\omega - \epsilon_\mathbf{k} + \mu_\sigma - \Sigma_\sigma' - i\Sigma_\sigma''\right]^{-1}/\pi$, which form the basis for our calculation of $n(\mathbf{k})$ and of the RF spectrum using (1).

(I) Let us first discuss a simple self-consistent approximation [8], motivated by an analysis that reproduces the essentially exact result [13] of single $\downarrow$ spin ($n_\downarrow = 0$ limit) interacting with a Fermi sea of $\uparrow$ fermions [12]. We will show that this scheme has serious qualitative problems for $n_\downarrow > 0$ and analyze why this is the case. In this approximation, the Green's functions used to calculate Γ and Σ are the bare G's but with a *renormalized* chemical potential. A self-consistency condition is then imposed so that $\mu_\downarrow = \epsilon_{F\downarrow} + \Sigma_\downarrow'(k_{F\downarrow}, 0; \mu_\downarrow)$, where $\Sigma_\downarrow'$ itself depends on $\mu_\downarrow$ [13]. For the single minority spin limit, this reproduces the result $\mu_\downarrow(n_\downarrow = 0) = -E_b \simeq -0.6\epsilon_{F\uparrow}$.

This approximation for $n_\downarrow > 0$ implies the use of a *negative* $\mu_\downarrow$ in the bare $G_\downarrow$ used in Γ and Σ. As a result, one misses all effects of finite $n_\downarrow$ occupancy "inside" the calculation. We can then analytically see that $\text{Im}\Gamma(\mathbf{q}, \omega < 0) \equiv 0$ which impacts the results as follows.
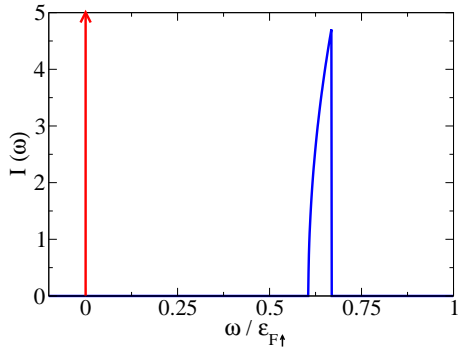
FIG. 1: (color online) RF spectrum of a unitary Fermi gas with $n_\downarrow/n_\uparrow = 0.25$ calculated within the self consistent approximation (I) (see text). The majority ($\uparrow$, red) is a delta function with weight $n_\uparrow$. The minority ($\downarrow$, blue) spectrum has a discontinuity and a shift due to interactions, but no high frequency tail.
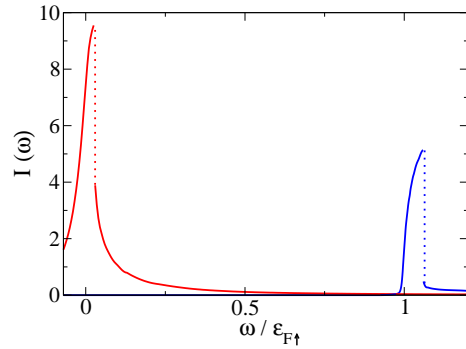

FIG. 2: (color online) RF spectra of a unitary Fermi gas with $n_\downarrow/n_\uparrow = 0.05$ within a simple ladder approximation (II) (see text). Both minority ($\downarrow$, blue) and majority ($\uparrow$, red) spectra exhibit a discontinuity (dashed) and a large-ω tail. The blue curve for minority spins is $15 \times I_\downarrow(\omega)$.

For the minority fermions $\Sigma''_\downarrow(\mathbf{k}, \omega < 0) \equiv 0$, which implies $A^{\text{inc}}_\downarrow(\mathbf{k}, \omega < 0) \equiv 0$ and thus $n_\downarrow(\mathbf{k}) = Z_\downarrow \Theta(k_{F\downarrow} - k)$. This means that $\sum_\mathbf{k} n_\downarrow(\mathbf{k}) = Z N_\downarrow < N_\downarrow$ and the zeroth moment sum rule for $I_\downarrow(\omega)$ is violated. In addition, in the absence of any incoherent spectral weight for $\omega < 0$, one also misses both the universal k^{-4} tail in $n_\downarrow(\mathbf{k})$ and the $\omega^{-3/2}$ tail in the RF spectrum (see Fig. 1). The first moment of $I_\downarrow(\omega)$ is then finite, instead of diverging as it should. Further, the majority spins are *completely unaffected by interactions* in this approximation since one can see analytically that $\Sigma_\uparrow(\mathbf{k}, \omega) \equiv 0$, which is clearly unphysical for non-zero $n_\downarrow$. The majority ($\uparrow$) RF spectrum is thus a delta function, a result that is at odds with all available experiments. Clearly this approximation fails to provide a reasonable description of RF spectra of highly imbalanced gases, despite its success in obtaining reasonable numerical estimates for $\mu_\downarrow$. All of the problems here arise from the fact that propagators with renormalized $\mu_\downarrow < 0$ are used *without* taking into the shifts in the $\downarrow$ particle dispersion.

(II) This suggests that it may be physically more sensible to do the simplest calculation *without* any attempts at partial self-consistency, i.e., evaluate all diagrams with bare propagators and bare $\epsilon_{F\sigma}$. This leads to equations which are identical with the $1/N$ approximation [15] with $N = 1$ at the end. Now, in contrast to the previous approximation, the p-p vertex $\text{Im}\Gamma$ has structure even for $\omega < 0$, and this leads to $n(\mathbf{k})$ and $I(\omega)$ with universal tails for both spins.

Our numerical results for the RF spectra of a highly polarized unitary Fermi gas with $x = n_\downarrow/n_\uparrow = 0.05$ are shown in Fig. 2. Both majority and minority spectra show jump discontinuities and high frequency tails. The spin-independent $\omega^{-3/2}$ behavior tails are observed in Fig. 3. Comparing the results of (I) the self-consistent μ_σ approximation in Fig. 1 and (II) the simplest ladder
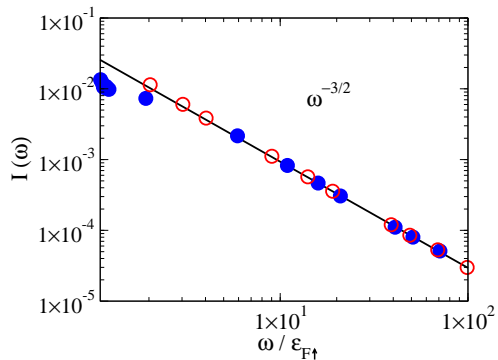

FIG. 3: (color online) High frequency tails of the RF spectra of the unitary Fermi gas with $n_\downarrow/n_\uparrow = 0.05$ shown in Fig. 2. Both majority (red, open circles) and minority (blue, filled circles) spectra exhibit a $\omega^{-3/2}$ tail.

approximation in Figs. 2 and 3, there is no doubt that the latter provides a far better qualitative description of the RF spectrum.

Despite these qualitative successes, it must be emphasized that the simple ladder approximation (II) is not quantitatively accurate insofar as the calculated chemical potentials, e.g., $\mu_\downarrow = \epsilon_{F\downarrow} + \Sigma'_\downarrow(k_{F\downarrow}, 0; \epsilon_{F\downarrow})$. In particular we find that in the single spin limit $\mu_\downarrow(n_\downarrow = 0) \simeq -0.9\epsilon_{F\uparrow}$, as compared with the exactly result of $-0.6\epsilon_{F\uparrow}$. Moreover, we have found that the simple ladder approximation leads to a negative compressibility for $x \gtrsim 0.05$ clearly signaling the limitations of the approximation.

The prospects for a better diagrammatic approximation are unclear, since fully self-consistent calculations do not necessarily lead to better answers in strongly interacting systems [23]. We also note that, while Quantum Monte Carlo (QMC) calculations have often provided valuable quantitative information[12] for energet-

ics, extracting frequency-dependent correlation functions from QMC is very difficult in view of two serious issues: the fermion sign problem in polarized systems and the problem of analytic continuation.

Comparison with Experiments: Let us begin with the universal high frequency tail. A long tail is visible in all of the published spectra (Fig. 1 of ref. [5]; Fig. 2 of ref. [6]). It is present for superfluid as well as normal state spectra and the same for both spin species, as we predict. It would be interesting to know if the signal to noise ratio in experiments is sufficient to test the $3/2$ power law [24] and determine the coefficient C [17].

The jump discontinuity in the $T = 0$ RF signal for a normal Fermi liquid will be broadened by finite temperature and by experimental resolution. The best we can expect then is to see a peak at, or very close to, the location of the discontinuity. For the minority spins eq. (4) predicts this to be $\omega_\downarrow^*/\epsilon_{F\uparrow} = 3A_0/5 - (1 - m/m_0^*)x^{2/3} - 6Fx/5$, using the best QMC result [25] for $\mu_\downarrow$. This is exactly the expression used for the peak position by Schirotzek *et al.* [6]. For the majority spins, with $m^* \simeq m$, the peak will be at $\omega_\uparrow^*/\epsilon_{F\uparrow} = 2A_0x/5 + Fx^2/5$, which is slightly shifted from zero.

Conclusions: We have derived two exact results for singular features in the RF spectra of Fermi gases. The high frequency $\omega^{-3/2}$ is a universal feature, independent of the nature of the many-body state, when final state interactions are negligible, and provides an opportunity for measuring Tan's contact C. Such a study combined with other experimental probes such as photoassociation [26] could provide deeper understanding of how short range physics controls the universal properties of strongly interacting cold gases. Our second exact result on the jump discontinuity in the spectrum of a Fermi liquid at $T = 0$ provides a distinguishing feature between a normal and superfluid ground state. In the second part of our paper we show that, in the absence of a small parameter, it is very difficult to obtain reliable results for the detailed frequency dependence of the RF spectra – which capture both general qualitative features and are quantitatively accurate – in strongly interacting quantum gases. Indeed, that makes exact results such as sum rules and the singular features derived in this paper all the more important in interpreting experiments.

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